

Fast Monte Carlo simulations and singularities in the probability distributions of non-equilibrium systems

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A numerical technique is introduced that reduces exponentially the time required for Monte Carlo simulations of non-equilibrium systems. Results for the quasi-stationary probability distribution in two model systems are compared with the asymptotically exact theory in the limit of extremely small noise intensity. Singularities of the non-equilibrium distributions are revealed by the simulations.

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The understanding of fluctuations in systems away from thermal equilibrium is a problem of long standing in statistical physics [1]. Well known examples of physical phenomena in which non-equilibrium fluctuations play a particularly important role include e.g. switching of polarization in lasers [2], switching between different configurations in proteins [3], the transition to instability in Josephson junctions [4], and chemical reactions [5].

In non-equilibrium systems, where symmetries of detailed balance are broken, no general methods exist for the calculation of even basic quantities like the probability distribution. This is a case where numerical and asymptotic theoretical methods for investigating the probability distribution are of particular importance.

Theoretical approaches, such as WKB-like or path-integral methods, are available in the limit of small noise intensity, $D \rightarrow 0$ [5, 6, 7, 8]. In particular the theory suggests that a solution to the problem of non-equilibrium fluctuations requires an understanding of the dynamics of deviations from the steady state [1] and an analysis of singularities in the non-equilibrium potential [11, 12]. Some ideas about how to extend the existing ($D \rightarrow 0$ limit) theory for still small but finite noise intensities have recently been suggested [9, 10, 20].

The main numerical technique used to verify theoretical predictions, and to analyse the behavior of the dynamical system under study, is Monte Carlo simulation. The theory gives an asymptotically exact solution in the $D \rightarrow 0$ limit. In contrast, D in the numerical simulations is necessarily finite. Typically, the time required for Monte Carlo simulations grows exponentially as $D \rightarrow 0$. This meant that theoretical predictions of interesting singular structures, and of the non-equilibrium probability distribution [11, 13], for long remained untested either experimentally or by numerical simulation. Moreover there was no clear understanding of how the picture changes for small but still finite noise intensities.

Approaches that have been tried to speed up the simulations have focused mainly on finding optimal fluctuational paths and rates of transition between stable states of a system (e.g. efficient transition path sampling [14] and dynamics importance sampling [15], following the earlier suggestion of [16]). In [17] the path sam-

pling method was adapted for non-equilibrium systems. Based on the same idea, the umbrella sampling technique was suggested to estimate the probability of reaching any point in the phase space of an equilibrium system starting from a fixed initial state [14]. A technique for improving sampling in equilibrium systems by splitting up the probability packets was introduced in [18]. So far, however, no general algorithm has been suggested, able to give both the whole probability distribution and dynamical information like the optimal fluctuational paths for small noise intensities for non-equilibrium systems.

In this Letter we introduce a numerical method that enables the time required for Monte Carlo simulations to be reduced by an exponentially large factor. It is applicable to generic two-dimensional non-equilibrium systems, does not require any *a priori* knowledge about the system apart from its dynamical equations of motion, and it allows the quasi-stationary probability distribution to be computed directly over the whole phase space. Using this method, we reveal for the first time singular behavior of the non-equilibrium distribution in numerical simulations, and we show that the results are in quantitative agreement with the asymptotic theory.

The central idea is to perform the simulations in sequential steps. We construct the quasi-stationary distribution, patching together intermediate results: we start from one of the steady states and gradually move away from it. We find that the time required for the simulations at each step is reduced by an exponentially large factor as compared to the standard technique: if the time necessary for a conventional Monte Carlo simulation technique is T , our modified method would require only time $T_m \approx NT \exp^{-(N-1)\frac{\Delta\Phi}{D}}$, where N is the number of steps involved and $\frac{\Delta\Phi}{D}$ is their separation in terms of the logarithm of the probability [24].

We first explain the method on a very simple equilibrium stochastic system, and then we apply it to two much-studied non-equilibrium systems and compare the numerical results with theoretical predictions. To illustrate the technique, we consider an overdamped Brownian particle moving in a bistable Duffing potential $U(x) = -x^2/2 + x^4/4$

$$\dot{x} = -U'(x) + \xi(t), \quad (1)$$

where $\xi(t)$ is zero-mean white Gaussian noise with intensity D and moments

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(0) \rangle = 2D\delta(t).$$

The probability distribution is completely defined by the potential $U(x)$, and is of the Boltzmann form $\rho(x) \propto \exp(-U(x)/D)$. As in the case of a non-equilibrium system (where the probability distribution is not defined by a potential) a standard Monte Carlo technique can be used to deduce $\rho(x)$. Numerical integration [19] of the Langevin equation (1), assuming the system to be located initially at one of the potential minima x_m , gives the discrete probability distribution $\rho(x)$, peaked at x_m . The potential can be deduced as $\Phi(x) \propto -D \ln \rho(x)$. If the noise intensity is very small, the system fluctuates in a close vicinity of x_m and large deviations from it are extremely rare. Accordingly, the conventional Monte Carlo technique cannot be used to study the dynamics of optimal escape paths, or the properties of the probability distribution far from the potential minima: for small noise intensities the statistics required cannot in practice be collected within a realistic time.

In order to overcome this problem, we start from the distribution already obtained near x_m . We fix two probability levels ρ_i and ρ_f , lying well within the region where the numerical ρ is accurate, with $\rho_f < \rho_i$ corresponding to two levels in the potential Φ_i and Φ_f , and two coordinates x_i and x_f , as shown in Fig. 1. We require the levels ρ_i and ρ_f to be fairly different, such that the corresponding x_i and x_f are sufficiently separated: the distance between them must exceed \sqrt{Dh} , where h is the integration time step used in the Monte Carlo simulation, and must also exceed the discretization step Δx in the discrete probability distribution.

The next step of the simulation is started from the level Φ_i (putting the system at $x = x_i$ as its initial condition). If the system starts to evolve along a fluctuational trajectory (towards the boundary of attraction) we just follow its natural dynamics according to (1) and collect the statistics for building the probability distribution in the usual way. If the system starts with a relaxation trajectory (towards x_m), or when it crosses the boundary x_i due to relaxation some time later, we stop the simulation and reinject the system back to the initial state x_i . In this way we simulate the full dynamics of the system at higher levels of the potential $\Phi(x) > \Phi_i$ (in the region of coordinate space $x > x_i$ for this particular case). Thus, in the subsequent simulation step we follow only those fluctuations that have already attained a certain level in the potential Φ_i , without waiting for this exponentially slow event to happen. In this way, a new piece of the probability distribution is built with a time saving $\sim \exp \Phi_i/D$ compared to a simulation starting from the potential minimum x_m . The computed new piece of the potential $\Phi_2(x)$ is shown as the upper curve in Fig. 1.

The two pieces of the inferred potential (the original $\Phi_1(x)$ and the new $\Phi_2(x)$) are then merged at x_f by a simple shift. Continuing this procedure, the probability

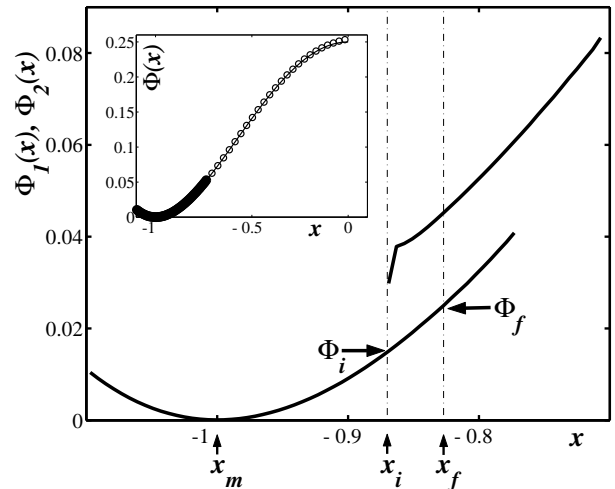


FIG. 1: The first ($\Phi_1(x)$, lower curve) and second ($\Phi_2(x)$, upper curve) pieces of the inferred potential $\Phi(x)$ for the system (1) with $D = 0.005$. The discontinuity in the gradient of $\Phi_2(x)$ near x_i is an artefact due to a boundary effect in the calculation of the discrete probability distribution. To avoid this problem $\Phi_1(x)$ and $\Phi_2(x)$ are merged at the point x_f and the initial part of $\Phi_2(x)$ is discarded. We normalize $\Phi_1(x)$ choosing $\Phi_1(x_m) = 0$, and each successive piece of $\Phi(x)$ is normalized in order to match with the previous one at the point where they join. Inset: the inferred potential $\Phi(x)$ for the system (1) with $D = 0.005$. The new technique (circles) is compared with standard Monte Carlo simulations (bold line) and with the Duffing potential $U(x)$ (thin line).

distribution and the corresponding potential can be built, step by step, for the whole region of interest. The inset in Fig. 1 shows the resultant potential, built from 13 such pieces between the minimum at $x_m = -1$ and the maximum at $x = 0$. It coincides closely with the Duffing potential $U(x)$ itself. The potential $\Phi(x)$ is thus inferred within a region of coordinate space that is inaccessible in a conventional simulation (shown as bold curve for comparison). We stress that no *a priori* knowledge of the dynamics has been used in the simulations, and that the method is robust to choice of parameters.

In the case of a two dimensional system, the procedure remains essentially the same. The main difference is that, instead of identifying two points x_i and x_f , we need to identify two closed lines of constant probability. One line is a boundary line for starting simulations from, and the other is a reference line for matching together different pieces of the probability distribution (see Fig.2 for clarification) [25]. The crucial point of our technique is that, in starting the simulations from the boundary line, we must not perturb the natural dynamics of the system. This implies that we should consider the reinjection location probability (RLP) along the boundary line corresponding to ρ_i . Starting from the second step of the simulations, the system should be reinjected back according to the RLP after it relaxes across the boundary. We emphasize that the RLP is not the same as

the probability distribution $\rho(\mathbf{x})$, which is constant on the boundary line. The RLP is an additional important measure which describes local discrete dynamics in the neighborhood of the boundary line. It is a distribution along the boundary of how often the system crosses it.

In an equilibrium system, detailed balance provides a symmetry that can be used to reinject the system back at the boundary level, without any need to compute the RLP. For non-equilibrium systems, however, this procedure is inapplicable. The RLP should be considered separately (and calculated explicitly) for the particular system being investigated. It can be obtained from an analysis of the finite difference equation corresponding to the model. In the limit of small integration time step the probability to cross the boundary is proportional to the diffusion-related term in the finite difference equation. Then the RLP is simply proportional to the projection of the vector orthogonal to the boundary onto the coordinate affected by the noise ξ . It can also be computed numerically.

For non-equilibrium systems, the limit of small noise intensity is of particular importance. A sufficiently small D gives rise to the possibility of revealing the non-equilibrium potential

$$\Phi(\mathbf{x}) = \lim_{D \rightarrow 0} -D \ln \rho(\mathbf{x}),$$

directly through a numerical experiment. Observations of the predicted singular shape of $\ln \rho(\mathbf{x})$, and of its dependence on D , are thus of considerable interest.

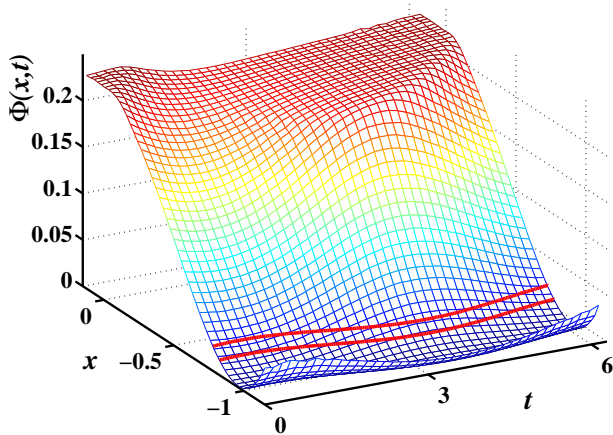


FIG. 2: The whole inferred $\Phi(x, t)$ for the system (2) for $A = 0.1$, $\Omega = 1$, $D = 0.005$. Two lines are the lines of constant probability found after the first step of simulations. The corresponding levels of probability were chosen as $\Phi_i = 3D$ and $\Phi_f = 5D$.

As a first example of a nonequilibrium system, consider the periodically-driven overdamped Duffing oscillator

$$\dot{x} = -U'(x) + A \cos \Omega t + \xi(t). \quad (2)$$

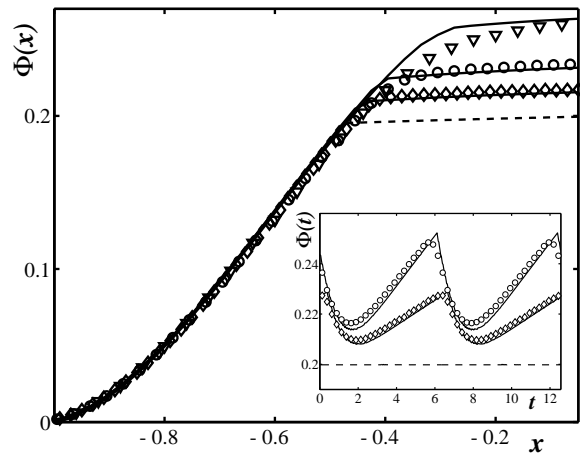


FIG. 3: A time section of the inferred $\Phi(x, t = 4.1)$ for the system (2) with $A = 0.1$, $\Omega = 1$, and different noise intensities: $D = 0.005$ (diamonds); $D = 0.01$ (circles); and $D = 0.02$ (triangles). The theoretical predictions are shown by full lines for finite noise intensities, and by dashed line for $D = 0$. Inset: oscillations of $\Phi(x, t)$ at the boundary of attraction for different noise intensities.

We infer $\Phi(x, t)$ as $-D \ln \rho(x, t)$. This quantity corresponds to the theoretical “global minimum of the modified action” in the Hamiltonian theory of large fluctuations [20] and, in the limit $D \rightarrow 0$, it becomes the non-equilibrium potential.

The complete $\Phi(x, t)$, constructed from 12 such pieces, is shown in Fig. 2 and a time section of $\Phi(x, t)$ calculated for different noise intensities together with the results of theoretical calculations (Hamiltonian theory including the prefactor) [20] is shown in Fig. 3. The RLP in the simulations can be taken as constant if a small enough integration time step is used in the scheme. A small difference between the theory and the simulations results appears for larger noise intensities then the asymptotic theory starts to break down.

As a second, more complicated, nonequilibrium example, consider the inverted Van-der-Pol oscillator

$$\ddot{x} + 2\eta(1 - x^2)\dot{x} + \omega_0^2 x = \xi(t) \quad (3)$$

Here, in order to be able to merge more easily the different pieces of $\Phi(x, y)$, we apply a coordinate transformation from x and $y = \dot{x}$ to amplitude A and phase ϕ ($x = A \cos(\phi)$, $y = -A\omega_0 \sin(\phi)$). The probability $\rho(x, y)$ can be then analyzed in the (A, ϕ) coordinate space. This makes the problem very similar to the periodically driven Duffing oscillator: the only difference is the RLP which, in the case of the Van der Pol oscillator, turns out to be strongly modulated. It is essential for this modulation to be taken into account when reinjecting the system back to the boundary of constant probability. Two sections of $\Phi(x, y)$, obtained from the simulations for different parameters η , are compared with the theory in Fig. 4. Again, the agreement between numerics and theory is excellent.

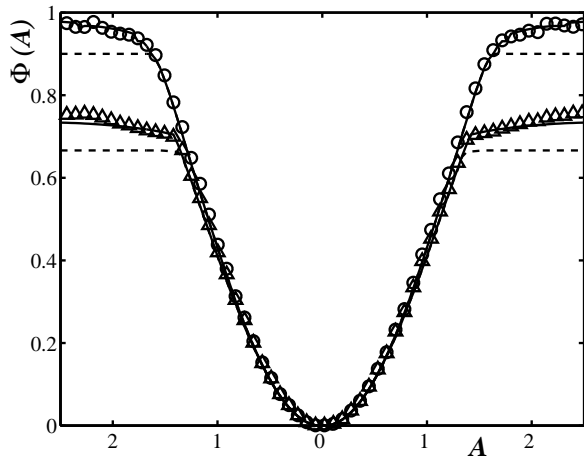


FIG. 4: A section ($x = y$) of the inferred $\Phi(A)$ for the system (3) with $\omega_0 = 1$, noise intensity $D = 0.01$ and $\eta = 0.25$ (circles); and $\eta = 0.5$ (diamonds). Theoretical predictions are shown in each case for $D = 0$ (dashed curves) and $D = 0.01$ (full curves).

The non-equilibrium systems considered in this Letter share the same structure of singularities. Using the fast Monte Carlo simulations we reveal plateaus, the essentially flat regions in the probability distribution, which can be observed close to boundaries of attraction. They result from a purely dynamical effect that is not associated with the flatness of any potential. We have shown

that its origin is related to switching between different types of optimal fluctuational path, and it is a general feature of non-equilibrium systems with metastable states [20, 21]. The switching lines [12] are revealed as lines along which the “global minimum of the modified action” $\Phi(\mathbf{x})$ exhibits sharp bends – corresponding to the predicted line at which the non-equilibrium potential is non-differentiable. In the boundary region we found the oscillations of the probability distribution and their dependence on noise intensity (see the inset in Fig.3) discussed in the recent publications [9, 10, 22]. Using the simulations we demonstrated noise induced shift of the singularities and the optimal escape path, which has stimulated a new step in the development of the theory [20].

We emphasize that the singularities can be confidently observed only in the limit of extremely small noise intensity, and therefore that the use of our new technique is crucial in that it reduces by an exponentially large factor the time required for Monte Carlo simulations. In addition to being fast, it preserves dynamical information, can be modified to analyse optimal fluctuational paths, is applicable to the energy-optimal control problem [23], and can be further extended to encompass higher dimensional systems and maps.

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 - [24] It is illuminating to compare simulations of the Duffing system by the fast and conventional techniques: the results of Fig. 3 took us ~ 15 minutes to simulate with $D = 0.02$, whereas for the same noise intensity it takes ~ 4 days of standard Monte Carlo simulation to obtain comparable statistics close to the boundary of attraction.
 - [25] In the case of an N -dimensional system, this would correspond to $(N - 1)$ -dimensional surfaces of constant probability dividing the phase space into separate regions.